

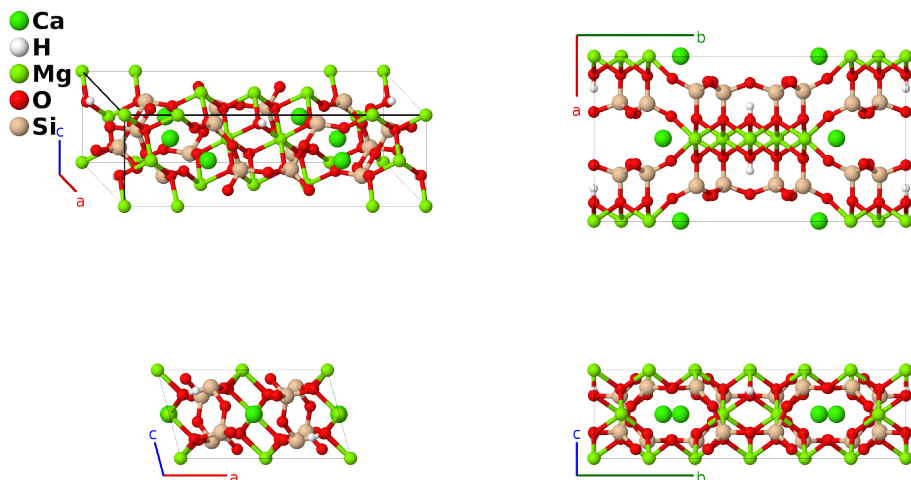
Tremolite ($\text{Ca}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ S_4_2) Structure: A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j-001

This structure originally had the label A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/BQ7Y>

https://aflow.org/p/A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j-001



Prototype	$\text{Ca}_2\text{H}_2\text{Mg}_5\text{O}_{24}\text{Si}_8$
AFLOW prototype label	A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j-001
<i>Strukturbericht</i> designation	S_4_2
Mineral name	tremolite
ICSD	none
Pearson symbol	mC82
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j-001 --params=a, b/a, c/a, β, y_2, y_3, y_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}</pre>

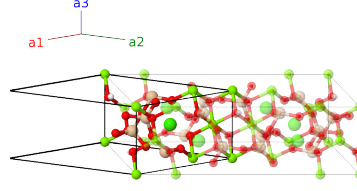
Other compounds with this structure

$\text{Ca}_2\text{H}_2(\text{Mg}_{5-x}, \text{Fe}_x)\text{O}_{24}\text{Si}_8$, $\text{Ca}_2\text{F}_2\text{Mg}_5\text{O}_{22}\text{Si}_8$

- There is no entry for (Merli, 2000) in the ICSD or CCDC, but the CIF can be downloaded from the American Mineralogist Crystal Structure Database.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Mg I
\mathbf{B}_2	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(4g)	Mg II
\mathbf{B}_3	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-by_2 \hat{\mathbf{y}}$	(4g)	Mg II
\mathbf{B}_4	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Ca I
\mathbf{B}_5	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Ca I
\mathbf{B}_6	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Mg III
\mathbf{B}_7	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Mg III
\mathbf{B}_8	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	H I
\mathbf{B}_9	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	H I
\mathbf{B}_{10}	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
\mathbf{B}_{11}	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
\mathbf{B}_{12}	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_{13}	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_{14}	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{15}	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{16}	$-(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{17}	$(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{18}	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{19}	$-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{20}	$-(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{21}	$(x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{22}	$(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	O V
\mathbf{B}_{23}	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	O V

$$\begin{aligned}
\mathbf{B}_{24} &= \begin{matrix} -(x_{10} - y_{10}) \mathbf{a}_1 - \\ (x_{10} + y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - \\ cz_{10} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O V} \\
\mathbf{B}_{25} &= \begin{matrix} (x_{10} + y_{10}) \mathbf{a}_1 + \\ (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O V} \\
\mathbf{B}_{26} &= \begin{matrix} (x_{11} - y_{11}) \mathbf{a}_1 + \\ (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VI} \\
\mathbf{B}_{27} &= \begin{matrix} -(x_{11} + y_{11}) \mathbf{a}_1 - \\ (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - \\ cz_{11} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VI} \\
\mathbf{B}_{28} &= \begin{matrix} -(x_{11} - y_{11}) \mathbf{a}_1 - \\ (x_{11} + y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - \\ cz_{11} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VI} \\
\mathbf{B}_{29} &= \begin{matrix} (x_{11} + y_{11}) \mathbf{a}_1 + \\ (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VI} \\
\mathbf{B}_{30} &= \begin{matrix} (x_{12} - y_{12}) \mathbf{a}_1 + \\ (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VII} \\
\mathbf{B}_{31} &= \begin{matrix} -(x_{12} + y_{12}) \mathbf{a}_1 - \\ (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - \\ cz_{12} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VII} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_{12} - y_{12}) \mathbf{a}_1 - \\ (x_{12} + y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - \\ cz_{12} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VII} \\
\mathbf{B}_{33} &= \begin{matrix} (x_{12} + y_{12}) \mathbf{a}_1 + \\ (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{O VII} \\
\mathbf{B}_{34} &= \begin{matrix} (x_{13} - y_{13}) \mathbf{a}_1 + \\ (x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si I} \\
\mathbf{B}_{35} &= \begin{matrix} -(x_{13} + y_{13}) \mathbf{a}_1 - \\ (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - \\ cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si I} \\
\mathbf{B}_{36} &= \begin{matrix} -(x_{13} - y_{13}) \mathbf{a}_1 - \\ (x_{13} + y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - \\ cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si I} \\
\mathbf{B}_{37} &= \begin{matrix} (x_{13} + y_{13}) \mathbf{a}_1 + \\ (x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si I} \\
\mathbf{B}_{38} &= \begin{matrix} (x_{14} - y_{14}) \mathbf{a}_1 + \\ (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si II} \\
\mathbf{B}_{39} &= \begin{matrix} -(x_{14} + y_{14}) \mathbf{a}_1 - \\ (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - \\ cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si II} \\
\mathbf{B}_{40} &= \begin{matrix} -(x_{14} - y_{14}) \mathbf{a}_1 - \\ (x_{14} + y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - \\ cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si II} \\
\mathbf{B}_{41} &= \begin{matrix} (x_{14} + y_{14}) \mathbf{a}_1 + \\ (x_{14} - y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} \end{matrix} & (8j) & \text{Si II}
\end{aligned}$$

References

- [1] M. Merli, L. Ungaretti, and R. Oberti, *Leverage analysis and structure refinement of minerals*, Am. Mineral. **85**, 532–542 (2000).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).